

Coarse grained dynamics of the freely cooling granular gas in one dimension

Mahendra Shinde,^{1,2,*} Dibyendu Das,^{3,†} and R. Rajesh^{4,‡}

¹*Beijing National Laboratory for Condensed Matter Physics,
Institute of Physics, Chinese Academy of Sciences, Beijing-100080, China*

²*Centre for Nonlinear Studies and the Beijing-Hong Kong-Singapore Joint Centre for Nonlinear and Complex Systems,
Hong Kong Baptist University, Kowloon Tong, Hong Kong, China*

³*Department of Physics, Indian Institute of Technology, Bombay, Powai, Mumbai-400076, India*

⁴*Institute of Mathematical Sciences, CIT campus, Taramani, Chennai-600113, India*

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We study the dynamics and structure of clusters in the inhomogeneous clustered regime of a freely cooling granular gas of point particles in one dimension. The coefficient of restitution is modeled as $r_0 < 1$ or 1 depending on whether the relative speed is greater or smaller than a velocity scale δ . The effective fragmentation rate of a cluster is shown to rise sharply beyond a δ dependent time scale. This crossover is coincident with the velocity fluctuations within a cluster becoming order δ . Beyond this crossover time, the cluster size distribution develops a nontrivial power law distribution, whose scaling properties are related to those of the velocity fluctuations. We argue that these underlying features are responsible behind the recently observed nontrivial coarsening behaviour in the one dimensional freely cooling granular gas.

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I. INTRODUCTION

Consider a collection of particles, initially distributed randomly in space, evolving in time through ballistic transport and inelastic collisions. Such a system has been studied extensively as a simple model of granular systems as well as a tractable model in nonequilibrium statistical mechanics [1–12]. At initial times, the system undergoes homogeneous cooling, the energy decreasing with time t as t^{-2} in accordance with Haffs law [13, 14]. In this regime, the particles remain homogeneously distributed with inter-particle spacing being the only relevant length scale. At times larger than a crossover time t_c , the system crosses over to an inhomogeneous clustering regime where the energy decreases as $t^{-\theta}$, where θ varies with dimension and is different from 2 in dimensions lower than the upper critical dimension. In this regime, there is a growing length scale \mathcal{L}_t , determined by the size of the largest cluster.

In one dimension, much more is known than in higher dimensions. Through an exact solution [4, 5] of the problem with coefficient of restitution set to zero (sticky gas), and extensive simulations [6] of the inelastic gas, it is known that $\theta = 2/3$. The sticky limit may also be mapped to the dynamics of shocks in the inviscid Burgers equation [15]. Recently, we showed that, when the coefficient of restitution depends on the impact velocity, then a new timescale t_1 further subdivides the inhomogeneous clustering regime into two sub-regimes [11, 12]. This was based on a study of the density–density and

the velocity–velocity correlation functions. For times $t_c < t < t_1$, these structure functions scale exactly as in the sticky gas, obeying what is known as the Porod law [16]. However, for times $t > t_1$, the inelastic gas deviates from the sticky gas limit and the correlation functions violate Porod law. In addition, the density distribution and inter-particle distance distribution develop into power laws that are qualitatively different from that seen in earlier times. We will refer to the two sub-regimes as the Porod and fluctuation dominated ordering regimes, respectively.

Although the macroscopic statistical quantities studied in Refs. [11, 12] establish that the Porod and the fluctuation dominated ordering regimes are distinct, they do not reveal how fluctuations start dominating beyond the time scale t_1 . It was speculated that the fluctuation dominated ordering regime should have an effective process of fragmentation that will compete with the otherwise strong effective aggregation. Whether coarse grained density clusters break up or remain coherently moving objects can be directly checked by studying their dynamics. In this paper, we study cluster dynamics, in particular effective fragmentation rates, and show that the ordering process gets disturbed beyond a certain timescale.

The second question is regarding the origin of the crossover timescale t_1 . Earlier this was shown to depend on a velocity scale δ associated with the coefficient of restitution [11, 12]. The coefficient of restitution is often modelled as a function of the relative velocity– rather than being a constant– such that collisions become near elastic for relative velocities smaller than δ . This property is consistent with experiments [17–19], required by theory [20], as well as essential in simulations to prevent inelastic collapse [2]. In this paper we demonstrate that the time t_1 is marked by the particle velocity fluctuations within density clusters becoming of the order δ .

*Electronic address: mahendra.statp@gmail.com

†Electronic address: dibyendu@phy.iitb.ac.in

‡Electronic address: rrajesh@imsc.res.in

Thus, it is not the typical velocities but rather the velocity fluctuations that matter for correlation functions. We also present a consistent scaling theory to understand the dependence of velocity fluctuations, fragmentation rates and cluster size distribution on the parameters δ , time t and cluster size m .

In Sec. II, we define the model, the quantities of interest, and give details of the simulation. In Sec. III, we present results from numerical simulations for velocity fluctuations, fragmentation rates and cluster size distribution. We develop a scaling theory which enables us to understanding the scaling of the above quantities in terms of two exponents. Sec. IV contains a summary and discussion of results.

II. MODEL AND DEFINITIONS

In this section, we define the microscopic model, and the quantities of interest. The model consists of a collection of N point particles of equal mass on a ring of length L . Each particle moves ballistically until it collides with another particle. The collisions conserve momentum, but are inelastic, such that when two particles with initial velocities u_i and u_j collide, the final velocities u'_i and u'_j are determined by

$$u'_{i,j} = u_{i,j} \left(\frac{1-r}{2} \right) + u_{j,i} \left(\frac{1+r}{2} \right), \quad (1)$$

where r is the coefficient of restitution. The coefficient of restitution is velocity dependent such that collisions become elastic when the relative velocity tends to zero. As mentioned in the introduction, this feature is consistent with experiments and theory, and often used in simulations to circumvent inelastic collapse. Our results will not depend on the detailed dependence of the coefficient of restitution on relative velocity: we therefore choose a convenient functional form [6, 7],

$$r(v_{\text{rel}}) = \begin{cases} r_0 & \text{if } v_{\text{rel}} > \delta, \\ 1 & \text{if } v_{\text{rel}} \leq \delta, \end{cases} \quad (2)$$

where δ is a velocity scale in the problem. The collisions are elastic for relative velocities smaller than δ . The particles are initially distributed randomly in space with their velocities drawn from a Gaussian distribution.

Starting from the above microscopic model, we desire to study emergent processes such as fragmentation and aggregation of a collection of particles. To this end, a coarse grained description has to be introduced, which we do as follows. Divide the ring into N equally sized boxes. Let the number of particles in the i^{th} ($i = 1, 2, \dots, N$) box be called the box density. We define a cluster to be a collection of contiguous boxes with non-zero box density surrounded by two empty boxes. The total number of particles in this cluster will be called the size of the cluster. Similar definition has been used elsewhere,

for example see [21]. In earlier papers [11, 12], we had studied velocity-velocity and density-density correlations using the coarse grained box density. However, a single particle moving across the boundary of a box results in change of density. To study clusters, any coarse graining should make sure that particles move significantly, i.e. by at least a box spacing (L/N) to cause a change in configuration. The above definition of a cluster has this property.

One of the quantities of interest in this paper is velocity fluctuations σ within a cluster. Let \mathbf{u}_c be the centre of mass velocity of a cluster, i.e., $\mathbf{u}_c = m^{-1} \sum_{i=1}^m \mathbf{u}_i$, where \mathbf{u}_i are the velocities of the particles constituting the cluster, and m is the size of the cluster. Then, the velocity fluctuations of that cluster is $\sigma(m, t) = m^{-1} \sum_{i=1}^m (\mathbf{u}_i - \mathbf{u}_c)^2$, where the summation is again over all the particles constituting the cluster. When σ is much smaller than u_c^2 , then the cluster is compact and stable with respect to the velocity fluctuations. However, if they are of same order, or if $\sigma \sim \delta^2$, then the cluster may start breaking apart. This effect can be captured by defining an effective fragmentation rate of a cluster, as described below.

In the space of cluster sizes, a stochastic dynamics may be defined, with rates for the different processes being determined from simulations. As the clusters evolve in time due to the entry and exit of particles into and out of a cluster, we ask what the rates of transition from a cluster size m to m' are. Let $W(m \rightarrow m'; t)$ be the rate at which a size m changes into a size m' at time t . If $N(m, t)$ is the number of clusters per unit lattice site of size m at time t , then its time evolution is described by an effective Master equation [22]:

$$\begin{aligned} \frac{dN(m, t)}{dt} &= \sum_{m'} W(m' \rightarrow m; t) N(m', t) \\ &\quad - \sum_{m'} W(m \rightarrow m'; t) N(m, t). \end{aligned} \quad (3)$$

If in a time interval Δt , the cluster size decreases, then the cluster is said to have undergone fragmentation. Thus, an effective fragmentation rate $W_f(m, t)$ of a cluster of size m at time t can be defined as

$$W_f(m, t) = \sum_{m' < m} W(m \rightarrow m'; t). \quad (4)$$

We note that, in the above, fragmentation is an emergent process, not defined apriori in the microscopic dynamics, unlike some other models of granular gas where fragmentation occurs on collision [23, 24].

We study the model by means of event driven molecular dynamics simulations [25]. In the simulations the number density N/L is fixed to be to one and the number of particles to be $N = 20000$. The results in the paper do not depend on the precise values of the parameters r_0 and δ , as long as δ is much smaller than initial velocity differences of adjacent particles. We use generic values

$\delta = 0.001, 0.002, 0.004, 0.008$, and $r_0 = 0.1$ in the simulations. The initial velocities are chosen from a Gaussian distribution with width 1. The data is typically averaged over 20000 – 30000 different initial conditions. All averages will be over space and different histories and will be denoted by $\langle \dots \rangle$. Also, we use reduced units in which all lengths are measured in terms of initial mean inter particle spacing and times in terms of initial mean collision time.

III. RESULTS

There are four velocity scales in the problem. First is the typical speed of a cluster which decreases in time as $t^{-1/3}$ [4, 6]. Second is the root mean square velocity fluctuations $\sqrt{\sigma}$ within a cluster (discussed in detail below). Third is δ , characterising the coefficient of restitution [see Eq. (2)], while the fourth corresponds to the initial velocity distribution. At large times, there is no memory of the initial velocity distribution, and it will play no role in the subsequent discussion. When the typical speeds become of order δ , then almost all collisions are elastic and energy does not decrease any more. We will denote the latter crossover time by t_2 . Clearly, $t_2 \sim \delta^{-3}$. It is possible that the velocity fluctuations scale with time differently from the typical velocity. If so, we have a possibility of a different crossover time which is marked by the velocity fluctuations becoming order δ .

We first characterise the velocity fluctuations σ . In Fig. 1, we show the variation of σ with time t for different values of δ and two values of cluster size m . For short times, σ is independent of δ , and after initial transients, decays in time as a power law, with the exponent independent of m and the prefactor dependent on m . At large times, σ deviates from the power law behaviour and is constant for a while. We argue that this crossover occurs when σ is of order δ^2 — velocity fluctuations and hence relative velocities are such that collisions within a cluster become near elastic. Elastic collisions tend to smoothen out density inhomogeneities. Therefore, clusters become less compact and fragmentation is initiated. The observations are mathematically summarised as

$$\sigma(t, \delta) \simeq \delta^2 f_1 \left(t \delta^{2/x_1} \right), \text{ fixed } m, \quad (5)$$

$$\sigma(t, m) \simeq f_2 \left(\frac{t}{m^{x_2/x_1}} \right), \text{ fixed } \delta, \quad (6)$$

where x_1, x_2 are scaling exponents and f_1, f_2 scaling functions such that $f_1(z) \sim z^{-x_1}$, $z \ll 1$, and $f_2(z) \sim z^{-x_1}$, $z \ll 1$. Thus, for fixed δ , $\sigma \sim m^{x_2} t^{-x_1}$ for initial times.

The exponents x_1, x_2 may be obtained from the data collapse of the data in Fig. 1 when scaled as in Eqs. (5) and (6). The scaled data is shown in Fig. 2(a) [Eq. (5)]

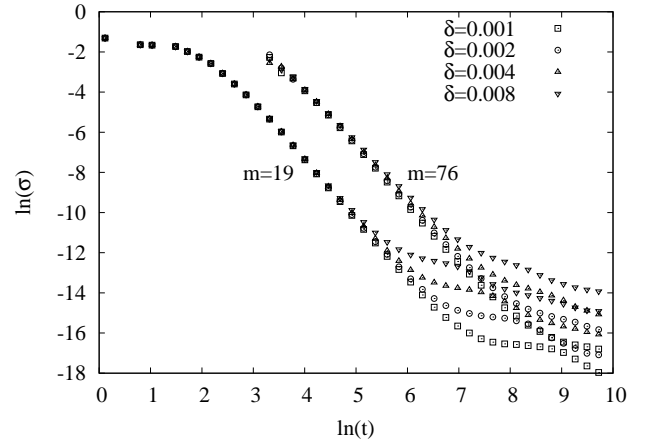


FIG. 1: The velocity fluctuations σ within a cluster of size m as a function of time t for different δ . The data are for sizes $m = 19$ and $m = 76$. For short times the curves, for a given size, decay as a power law and is independent of δ . Deviation from power law is seen earlier for larger δ .

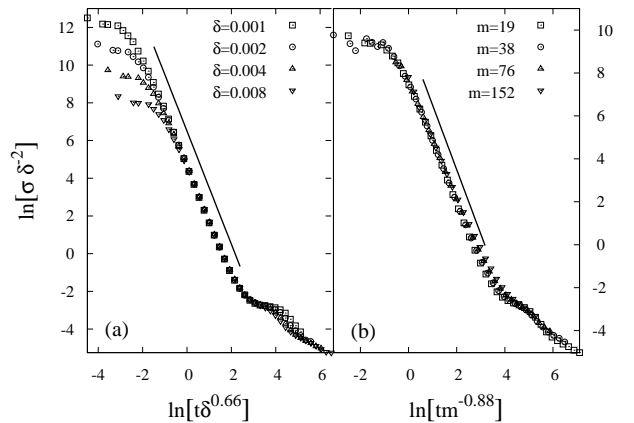


FIG. 2: Data collapse when scaled velocity fluctuations $\sigma \delta^{-2}$ is plotted against (a) scaled time variable $t \delta^{0.66}$ and (b) scaled time variable $tm^{-0.88}$. The data are for (a) $m = 19$ and (b) $\delta = 0.004$. The solid straight lines have slope = -3.0 .

and Fig. 2(b) [Eq. (6)]. From these, we obtain

$$x_1 = 3.00 \pm 0.06, \quad (7a)$$

$$x_2 = 2.66 \pm 0.08 \quad (7b)$$

Note that these values of x_1 and x_2 imply that the crossover time t_1 , relevant for σ , scales as $\delta^{-2/x_1} \sim \delta^{-0.66}$. This time scale is much smaller than $t_2 \sim \delta^{-3}$, which is the crossover time associated with velocities of nearly all particles becoming of order δ , i.e. all collisions becoming near elastic.

To contrast the above intra-cluster velocity fluctuations σ with typical cluster velocities, we study the centre of mass velocity \mathbf{u}_c of a cluster. It is well known that average energy per particle in the cooling gas decreases as

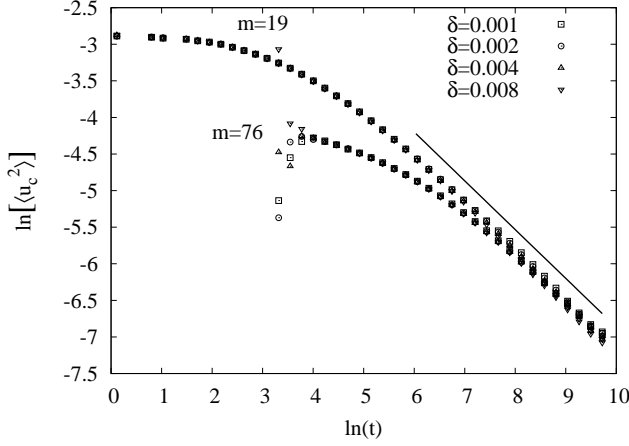


FIG. 3: The square of the centre of mass velocity $\langle u_c^2 \rangle$ of a cluster of size m as a function of time t for different δ . The data are for sizes $m = 19$ and $m = 76$. For the times shown, there is no dependence on δ . The solid line has slope $-2/3$.

$t^{-2/3}$ [6]. Not surprisingly, we find that the $\langle u_c^2 \rangle$ for a cluster decays with the same law. In Fig. 3, we show the variation of $\langle u_c^2 \rangle$ with time for different δ and two different cluster sizes. $\langle u_c^2 \rangle$ decreases as $t^{-2/3}$ at large t . There is no signature of any crossover across any intermediate time scale t_1 nor any dependence on δ . The intra-cluster near elastic collisions affect velocity fluctuations but not the typical speeds, which are affected only by cluster-cluster collisions.

We provide a further check for the exponent values in Eq. (7) by quantifying the velocity fluctuations σ_{\max} of the largest cluster in the system. From Eq. (6), we obtain that $\sigma_{\max} \sim M_{\max}^{x_2} t^{-x_1}$, where $M_{\max}(t)$ is the size of the largest cluster at time t . Noting that $M_{\max}(t) \sim t^{2/3}$ [4, 6], we obtain $\sigma_{\max} \sim t^{2x_2/3-x_1} \sim t^{-1.22}$, where we substituted the values of x_2 and x_1 from Eqs. (5) and (6). In Fig. 4, we show the variation of σ_{\max} with time t for different values of δ . The temporal regime which is independent of δ is consistent with the exponent 1.22.

We now show that the above crossover of σ from a power law is linked very closely to the initiation of fragmentation in clusters. The fragmentation rate $W_f(m, t)$ defined in Eq. (4) is numerically measured as follows. At time t , all the clusters of a particular size m are identified. At time $t + \Delta t$, the fraction of the identified clusters whose size has reduced is calculated. That fraction is equal to $W_f(m, t)\Delta t$. In the simulations, we choose Δt to be one, so that sufficient statistics may be obtained.

In Fig. 5, we show the fragmentation rate W_f for cluster size 19 for different values of δ . There is a sharp increase in the fragmentation rate, with the increase setting in earlier for larger δ . In the inset of Fig. 5, we superimpose the fragmentation rate on the plot of σ with time for the same value of δ and cluster size. Clearly, the increase in fragmentation rate coincides with the deviation from power law behaviour of the velocity fluctuations.

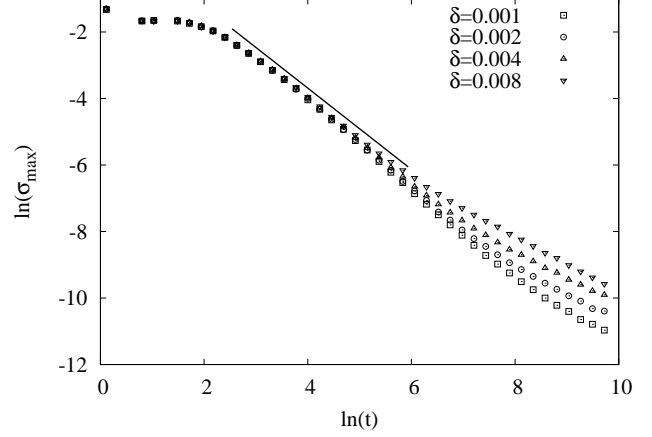


FIG. 4: The velocity fluctuations σ_{\max} of the largest cluster, as a function of time t for different δ . For short times the curves are independent of δ . Deviation from power law is seen earlier for larger δ . The solid straight line has slope -1.22 .

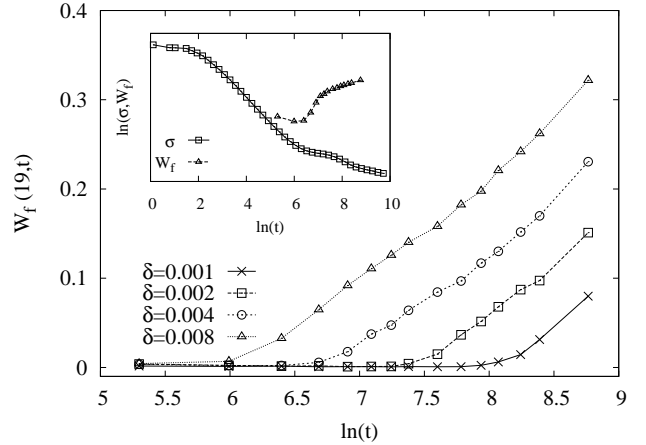


FIG. 5: Fragmentation rate W_f as a function of time t for different δ . The data are for cluster size 19. Inset: Velocity fluctuations σ and W_f as a function of time. Increase in fragmentation rate coincides with saturation of velocity fluctuations. The data are for $\delta = 0.004$ and cluster size 19.

This increased fragmentation rate results in fluctuation dominated coarsening and ultimately to the breakdown of Porod law [11].

The fragmentation rate W_f depends on the cluster size too. In Fig. 6, we show the variation of W_f with t for different m and fixed δ . The crossover time beyond which increased fragmentation is seen increases with m . Knowing that $t \sim m^{x_2/x_1}$ (Eq. (6)), we write

$$W_f(t, m) \simeq m^\eta f_w \left(\frac{t}{m^{x_2/x_1}} \right), \text{ fixed } \delta, \quad (8)$$

where η is an unknown exponent. We see that for $\eta = 0.5$, we obtain excellent data collapse [see inset of Fig. 6].

An increased fragmentation rate will result in clusters up to a size $m^*(t, \delta)$ breaking apart. We believe that this

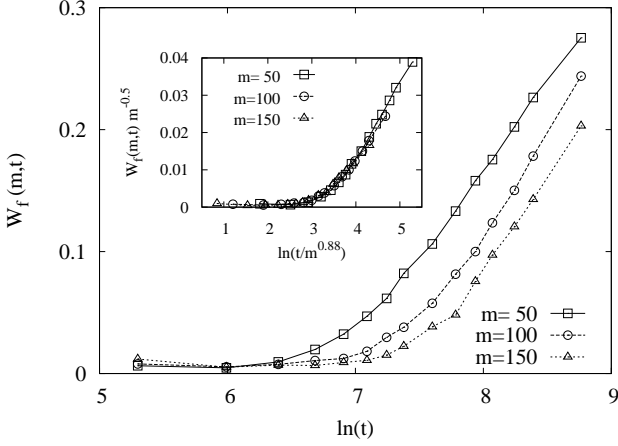


FIG. 6: Fragmentation rate W_f as a function of time t for different cluster sizes m . The data are for $\delta = 0.008$. Inset: Data collapse when W_f and time are scaled as in Eq. (8) with $\eta = 0.5$.

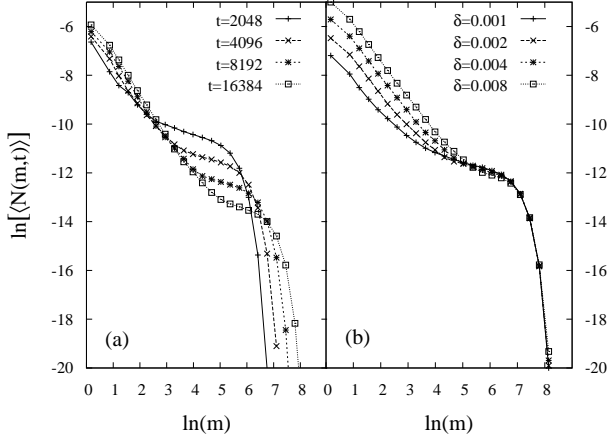


FIG. 7: The average cluster distribution $\langle N(m,t) \rangle$ as a function of cluster size m for (a) fixed $\delta = 0.004$, different times and (b) different δ , fixed time $t = 16384$.

is the origin of the breakdown of Porod law, as fragmentation results in new structures at small scales. One way to capture this is to study the average cluster size distribution $\langle N(m,t) \rangle$, where $N(m,t)$ is the number of clusters of size m at time t and the average is over space and histories. We would like to investigate whether, even in the presence of fragmentation, the cluster size distribution can be described by the sticky gas. We argue below that while some regimes of $\langle N(m,t) \rangle$ resemble the sticky gas, other regimes differ, but their scaling may be obtained from that of $\sigma(m,t)$. The mean cluster size distributions are shown for different times in Fig. 7(a) and for different δ in Fig. 7(b).

We note that for fixed time, $\langle N(m,t) \rangle$ for large masses has no dependence on δ [see Fig. 7(b)]. Thus, we expect that for masses greater than a mass cutoff $m^*(t, \delta)$, fragmentation is not relevant and $\langle N(m,t) \rangle$ should have

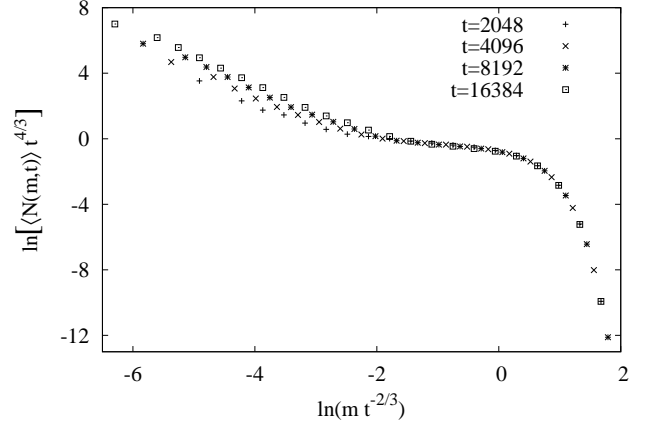


FIG. 8: Data collapse for large cluster sizes m when the cluster distribution $\langle N(m,t) \rangle$ and m are scaled as in Eq. (9). The data are for $\delta = 0.004$.

the same scaling behaviour as in the sticky gas. For the sticky gas, it is known [4] that

$$\langle N(m,t) \rangle \simeq \frac{1}{t^{4/3}} f_3\left(\frac{m}{t^{2/3}}\right), \quad (9)$$

where the scaling function $f_3(z) \sim z^{-1/2}$, $z \ll 1$ and $f_3(z) \rightarrow 0$ for $z \gg 1$. For masses $m > m^*(t, \delta)$ for which fragmentation is not important, we confirm numerically that the same scaling holds. In Fig. 8, we scale the data of Fig. 7(a) as in Eq. (9) and we see excellent data collapse for large cluster sizes, confirming that fragmentation can be neglected for cluster sizes larger than $m^*(t, \delta)$.

We note that in Fig. 8, there is no data collapse for small cluster sizes, when the data is scaled as in Eq. (9), and thus small cluster sizes cannot be described by the sticky gas scaling. We argue that its scaling can be obtained from that of the scaling of σ . For a fixed δ , varying t , $\langle N(m,t) \rangle$ should have the scaling form

$$\langle N(m,t) \rangle \simeq \frac{1}{t^\alpha} f_4\left(\frac{m}{t^{x_1/x_2}}\right), \quad m \ll m^*, \text{ fixed } \delta, \quad (10)$$

where α is an exponent which we determine by examining the large z behaviour of the scaling function $f_4(z)$. For large z , $f_4(z)$ should be such that it crosses over to the small z behaviour of $f_3(z)$. Thus $f_4(z) \sim z^{-1/2}$ for $z \gg 1$. Comparing the time dependence of Eqs. (9) and (10) in the latter limit, we obtain

$$\alpha = 1 + \frac{x_1}{2x_2} \approx 1.56. \quad (11)$$

The data when scaled as in Eqs. (10) and (11) with x_1 and x_2 as in Eq. (7) is shown in Fig. 9(a). We obtain good data collapse for the small cluster sizes, showing that knowing the scaling behaviour of σ helps us obtain the scaling behaviour of $\langle N(m,t) \rangle$. The small z behaviour of $f_4(z)$ can be determined numerically. We

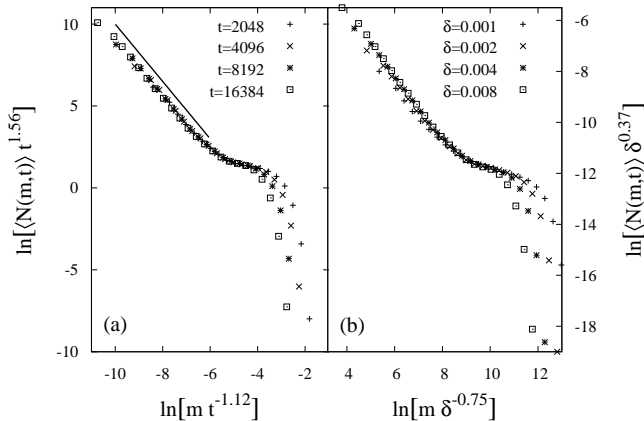


FIG. 9: Data collapse for small cluster sizes m when the cluster distribution $\langle N(m,t) \rangle$ and m are scaled as in (a) Eq. (10) for fixed $\delta = 0.004$ and (b) Eq. (12) for fixed $t = 16384$. The solid line has slope 1.75.

find that $f_4(z) \sim z^{-\tau}$ with $\tau = 1.75 \pm 0.08$ [see solid line in Fig. 8(a)].

The scaling of the small cluster sizes with δ can also be obtained from the scaling of σ . Knowing that m^* scales as δ^{2/x_2} , we write

$$\langle N(m,\delta) \rangle \simeq \frac{1}{\delta^\beta} f_5\left(\frac{m}{\delta^{2/x_2}}\right), \quad m \ll m^*, \text{ fixed } t, \quad (12)$$

where the exponent β can be determined as above by constraining the large z behaviour of the scaling function $f_5(z)$ to be the same as the small z behaviour of $f_3(z)$. This immediately implies that $f_5(z) \sim z^{-1/2}$ for $z \gg 1$ and

$$\beta = \frac{1}{x_2} \approx 0.37 \quad (13)$$

The data for cluster size distribution when scaled as in Eqs. (12) and (13) with x_1 and x_2 as in Eq. (7) is shown in Fig. 9(b). We obtain reasonable data collapse for the small cluster sizes. However, given the range and quality of data, it is possible to obtain data collapse for a range of x_2 .

IV. DISCUSSION

To summarise, we studied velocity fluctuations and size distribution of clusters in a freely cooling granular gas in one dimensional ring evolving via ballistic motion and inelastic collisions. The coefficient of restitution was $r_0 < 1$ for relative velocity greater than δ and 1 otherwise. The aim of the paper was to understand the consequences of a non-zero δ on the structure of clusters for large times.

For granular gases with realistic velocity dependent coefficient of restitution, it was recently shown [11, 12] that the nature of coarsening in the inhomogeneous cooling regime is not the same at all times. Beyond some

crossover scale t_1 , the coarsening behaviour changes at the macroscopic level from one that obeys Porod law to one that violates Porod law. These interesting numerical findings lacked a mesoscopic explanation of how and why the crossover occurs. The current paper provides an explanation. We demonstrate in this paper, that the transition from sticky gas regime to fluctuation dominated ordering regime within the inhomogeneous cooling regime may be viewed as a growing dominance of an underlying fragmentation process competing against the dominant clustering process. The fact that clusters break up is shown by the change of behaviour of the variance of particle velocities within a cluster. This crossover in velocity fluctuations coincide with an increase in the fragmentation rate of clusters leading to a richer fine structure reflected in the density-density correlations.

The velocity fluctuations within a cluster were found to decrease as a power law with time, with the velocity fluctuations being much smaller than the centre of mass velocities. However, when these fluctuations became of order δ , then intra cluster collisions became mostly elastic and the clusters start to fragment. This emergent phenomena was quantified by defining an effective fragmentation rate for a cluster. The fragmentation rate was seen to rise sharply at some cluster size dependent time with the crossover time increasing with decreasing δ . Once fragmentation sets in, the cluster size distribution $\langle N(m,t) \rangle$ changes drastically from that of the sticky gas ($r_0 = 0, \delta = 0$). However, the scaling of $\langle N(m,t) \rangle$ could be related to that of the velocity fluctuations $\sigma(m,t)$ which was completely characterised by two independent exponents x_1 and x_2 . It was also observed that the total energy of the system as well as clusters continue to decay as $t^{-2/3}$, showing no signature of the structural changes in the clusters.

We believe that many of these results (qualitative) will be carried over to higher dimensions. In two dimensions, for coarse grained velocities, it was shown [7] that the velocity fluctuations scale differently from the typical velocity. Hence, we expect a crossover when these fluctuations become comparable to δ , and thus fragmentation to be relevant for two dimensions too, and consequently a regime where coarsening is fluctuation dominated. It would be interesting to verify it numerically.

The velocity scale δ is relevant and not just a computational tool. Experimentally, $r(v)$ approaches 1 when the relative velocity v tends to zero, i.e., $r(v) \simeq 1 - (v/\delta)^\chi + \dots$, $v/\delta \ll 1$. The exponent χ takes a variety of values. Within the framework of viscoelastic theory, $\chi = 1/5$. Systems with $\chi < 1$ cannot be studied using event driven molecular dynamics simulations as inelastic collapse prevents the simulation from proceeding forward. It would be interesting to use conventional molecular dynamics simulations to verify whether the observations of this paper is valid for $\chi < 1$.

Another question of interest is the construction of lattice models that reproduce the coarse grained behaviour of the granular gas. Such models are not only computa-

tionally much faster, but also may be the first steps towards building effective field theories for the system. In a recent paper [26], a stochastic lattice model was studied which reproduced all features of the sticky gas. It would be interesting to see whether fragmentation can be incorporated into this lattice model such that the coarse grained behaviour seen in this paper is reproduced.

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